Available online at www.sciencedirect.com
ScienceDirect
Procedia Engineering 84 (2014) 920 – 926
Procedia Engineering
www.elsevier.com/locate/procedia

"2014 ISSST", 2014 International Symposium on Safety Science and Technology

Numerical simulation of three dimensional flow fields for extrusion process of GR-35 double-base propellant

ZHONG Tingting, RAO Guoning, PENG Jinhua*

Department of Safety Engineering, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

Abstract

Due to the instability of materials and the screw's rotation friction, it will be dangerous in the screw extrusion process of solid propellant. Because there were so much nitroglycerin and solid part in GR-35 double-base propellant, it was more difficult in spiral extrusion for this important propellant than others. In order to solve this problem, the Polyflow software was used to simulate the spiral extrusion process of GR-35 in this paper. Then four parameters (the temperature, the pressure, the shearing rate and the velocity) were analyzed at the axial direction (Z=0.02 m and Z=0.08 m). Then, these parameters of Z direction were analyzed by a line near the arris. According to the results, no matter the value of temperature, pressure, shearing rate or velocity, was larger in screw arris position. In addition, the values of temperature and pressure will increase as the extrusion processes while the velocity and the shearing rate will decrease. The simulated results can be used to optimize the technological in the process of screw extrusion of solid propellant and decrease the risks in process.

Peer-review under responsibility of scientific committee of Beijing Institute of Technology

Keywords: GR-35; screw extrusion; safety; polyflow; numerical simulation

Nomenclature

K	viscosity coefficient (Pa·s)
n	non-Newtonian index
p	pressure (Pa)
T	temperature of material (K)

* Corresponding author. Tel.: 025-84303182; fax: 025-84303182.
E-mail address: pengjh@njust.edu.cn

Peer-review under responsibility of scientific committee of Beijing Institute of Technology
doi:10.1016/j.proeng.2014.10.516

u	velocity ($m \cdot s^{-1}$)
ρ	density of material ($kg \cdot m^{-3}$)
τ	shearing stress, $N \cdot m^{-1}$
η	viscosity (Pa·s)
λ	relaxation time (s)
γ	shearing rate (s^{-1})

1. Introduction

There are many methods for molding process of solid propellant, such as extrusion method and casting method. In the large scale production of military industrial enterprises, the most commonly-used method is extrusion method, especially screw extrusion technology. There are many advantages for solid propellant produced by screw extrusion, such as stable performance, good inoxidizability, weather resistance and low-cost, etc [1]. But due to so much solid part and strong compression in extrusion process, the temperature will increase fast in actual production, which existed high risk and even lead to accidents. There was a statistic for 115 major accidents of solid propellant abroad. About 68% of these accidents occurred in production process [2]. So it is necessary to study the extrusion process of solid propellant for inherent safety. In the development of the solid propellant's screw extrusion process, it is essential to optimize the production process for higher quality of the solid propellant and producing safety. In recent years, some researchers had attempts to study the screw extrusion of the solid propellant by the extrusion theories in plastics, such as solid transportation theory, melting theory and melt conveying theory [3]. There were some useful results in their research, but there still exist potential problems to be solved.

Although there were two ways for extrusion process (single screw extrusion and twin-screw extrusion), the most common method was single screw extrusion. The single screw extruders were around 80% of all extruders in machinery industry of China [4]. This shows the important role of single screw extrusion. The single screw extruder was so important that many scholars focused on it. The research results of K.WilczyÄski [5] had revealed the performance of single screw extruder based on the simple model of single screw extrusion. In addition, from the perspectives of operating conditions, geometric features and barrel friction, Jaluria [6] had studied the solid transport model of screw. Besides, the discrete element method was used by M.R.Thompson [7] to simulate the flow of solid granules in screw extruder.

Polyflow is the fluid dynamics computational software by finite element method [8]. This software has enough capability to solve problems of nonlinear and non-Newtonian fluid, so it can be used to simulate the flow process of viscoelastic materials well. Because of its advantages, Polyflow applies to study screw extrusion of polymers and there were lot of examples for solving engineering problems by Polyflow software [9−10]. But there was little reference to study the extrusion process of solid propellants by Polyflow.

In this paper, Polyflow software was used to research the extrusion process of GR-35, one common solid propellant. GR-35 is one new type double base solid propellant. It contains about 35% nitroglycerin, some combustion catalysts and aluminum powder. Because of too much nitroglycerin and solid, it was difficult to spiral extrusion well in actual production [11]. To analyze the fluid field, the single screw extrusion process of GR-35 was simulated at the rotational speed of 20 $r \cdot min^{-1}$. Then the distributions of four parameters (temperature, pressure, viscosity and shearing rate) were calculated and analyzed under non-isothermal condition.

2. Numerical simulation

Due to the complexity of screw, there may be grid deformation during rotation process. So overlapping mesh method was used to overcome this difficulty when making mesh [12−13]. In this paper,the non-isothermal flow was studied, and the influence of viscosity on shearing rate was considered at the same time. So power law model [14] was used to calculate the parameters of non-isothermal flow under the constant heating and holding temperature.

2.1. Basic assumptions

In order to simulate one model well, two factors should be considered. The first one is in accordance with actual condition, and another one is the convenience of calculation. In view of the complexity between single screw extrusion process and all kinds of parameters, three assumptions for the characteristics of materials and technology features were listed as follows.

- The fluid is generalized non-Newtonian fluid and the flow pattern is laminar flow;
- The viscous force is much larger than inertia force and gravity, so inertia force and gravity can be ignored.
- The materials are both high viscosity and incompressible fluids, so the skidding between materials and barrels can be ignored.

According to above assumptions, the governing math equation, including equations of continuity and motion, can be established as follows [15−16].

$$\text{Continuity equations:} \quad \nabla \cdot \vec{u} = 0 \tag{1}$$

$$\text{Equations of motion:} \quad -\nabla p + \nabla \cdot \vec{\vec{\tau}} = 0 \tag{2}$$

According to the continuity of high polymer material during processing, as well as the conservation of momentum and energy, the power law model was used in this simulation.

$$\text{The power law model is} \quad \eta = K \cdot \left(\lambda \cdot \dot{\gamma} \right)^{n-1} \tag{3}$$

According the experimental data in reference [11], the unknown parameters in power law model can be determined by multivariate nonlinear regression. The results were listed in Fig. 1, and the values of K, n, λ were 296.23, 0.0998 and 1.714E^{-5}, respectively.

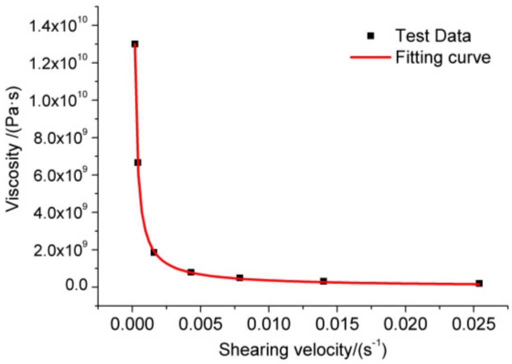

Fig. 1. The test results and fitting result of GR-35.

2.2. The simulation of solid propellant

Due to the complexity of screw model, a two-headed single screw was used to calculate in this paper. In order to decrease the requirement for computer and reduce the computation time, a screw with 100 mm in length was cut for simulation. This part contains one lead. The diameter of root screw is 70 mm and inner diameter of the cylinder is 100 mm. In addition, the distance between the screw arris and the cylinder is 9 mm. The finite element mesh in flow channel is hexahedron while the part of screw is tetrahedron. As shown in Fig. 2, the quality of mesh is good.

According the actual parameters of GR-35 in production process and the assumptions in 2.1, the Boundary conditions and material parameters of screw process were listed in Table 1.

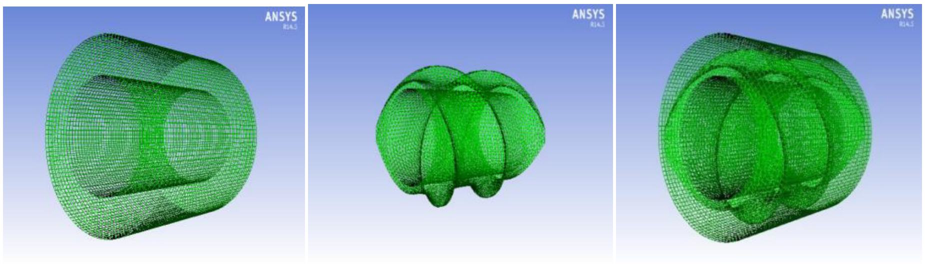

Fig. 2. Diagrams of making mesh.

Table 1. Boundary conditions and material parameters of screw process for GR-35.

Parameters	Stirring rate $r \cdot min^{-1}$	Inlet flow rate $m^3 \cdot s^{-1}$	Outlet pressure MPa	Heating temperature K	Holding temperature K	Average temperature K	Density $kg \cdot m^{-3}$	Specific impulse $N \cdot s \cdot kg^{-1}$
Value	20	$2*10^{-4}$	10	353	323	363	1600	2256

3. Results and analysis

To analyze the changes of four parameters well, two figures were given for every parameter. The first one is the distributions of four variables in *XY* section. The second one is a line closed to the arris, which listed the distribution at axial direction (*Y*=0). For all figures, the inlet was marked *Z*=0 m, while the outlet was *Z*=0.1 m.

3.1. Temperature

The temperature distribution trends of GR-35 in the process of extrusion were shown in Fig. 3 and Fig. 4.

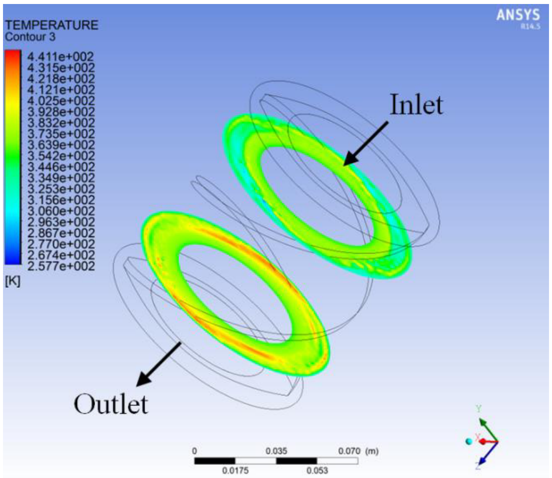

Fig. 3. Temperature distribution in XY section.

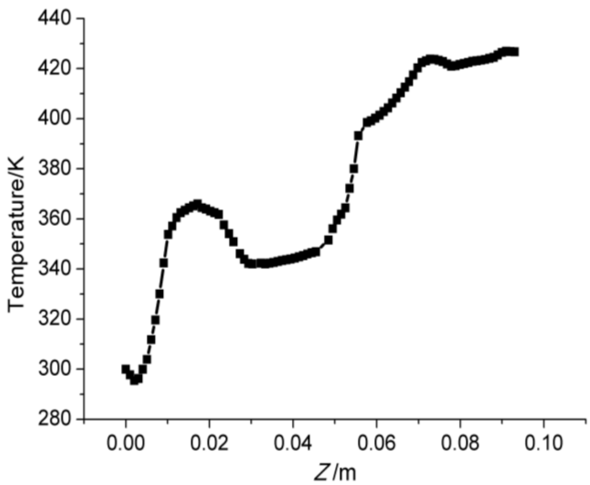

Fig. 4. Temperature distribution at axial direction.

The increase of temperature is the direct reason for burning and explosion hazard in the extrusion process. So, the variation of temperature is the most important aspect in the extrusion process. In other words, the reasonable temperature is an important parameter to ensure the safety of the propellant in the extrusion process. So the temperature distribution was listed in Fig. 4. It can be seen that the temperature was higher at the screw arris, the highest temperature was 430 K. This phenomenon may be caused by the friction and the mixture of propellant during rotating process of the screw. In addition, according to the results in Fig. 3, it can be seen that the temperature on the surface of the *Z*=0.08 m is more homogeneous and stable than the surface of the Z=0.02 m. Because the position of the *Z*=0.02 m is close to inlet, where carried the mixing process of the materials and relatively disordered, so the extrusion and deformation process of material is non-uniform. With the screw extruding, the process of mixing almost completely and the material become a steady-state situation.

According to Fig. 4, the temperature would increase at the screw arris and then decrease slowly, but the general trend was growing. The temperature can reach 370 K at the first arris (*Z*=0.015) and 425 K at the second arris (*Z*=0.07). This phenomenon was caused by heat transfer. In the position of arris, the hot water in the inner tube will heat the materials, but the materials will be cooling between two arrises by the cold water in the sleeve.

3.2. Velocity

The velocity distribution trends of GR-35 in the process of extrusion were shown in Fig. 5 and Fig. 6.

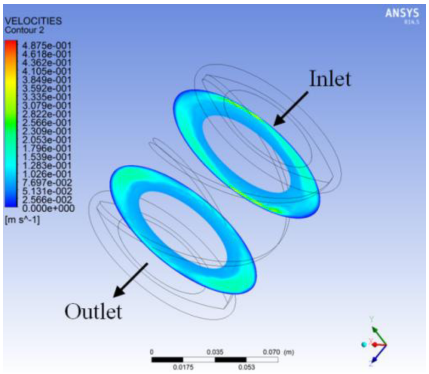

Fig. 5. Velocity distribution in XY section.

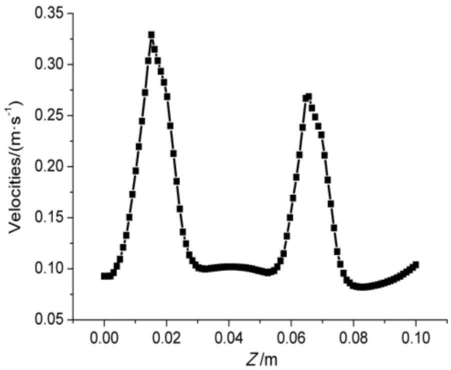

Fig. 6. Velocity distribution at axial direction.

The value of velocity can reflect the change of flux. As can be seen from Fig. 5 and Fig. 6, with the rotation of the screw, the rotational movement of materials will take place. The speed is relatively larger near the location of the screw arris. The velocity at the first screw arris is 0.33 $m \cdot s^{-1}$ (*Z*=0.015) and at the second arris is 0.26 $m \cdot s^{-1}$ (*Z*=0.07) . That's because there was small gap between the screw arris and the cylinder, and it lead to great velocity gradient. However, it reduced to 0.07 $m \cdot s^{-1}$ with the material mixing and extrusion process. As shown in Fig. 5, the velocity was low when materials closed to the cylinder wall because of no slip between material and the cylinder. When the rotate speed and the inlet flow rate was in certain circumstances, the speed will reduce from inlet to outlet. The large screw speed can make the material mixed well and squeeze tighter, so the speed of the material may decrease. That may lead to danger in the actual production. Therefore, it's necessary to select certain screw rotation to ensure extrusion process of the material normally and safety.

3.3. Shearing rate

The shearing rate distribution trends of GR-35 in the process of extrusion were shown in Fig. 7 and Fig. 8.

As can be seen from Fig. 7, as the continuous rotation of the screw, there were shearing stress to affect the material at the position of arris. The maximum shearing rate appeared clearly between the screw arris and cylinder in the process of the propellant's extrusion. Furthermore, the value of the shearing rate at the first arris is higher than that at the second. Based on the above results, the velocity reduction may lead to the reduction of shear rate, too. So the tendency of the shear rate is consistent with the velocity well.

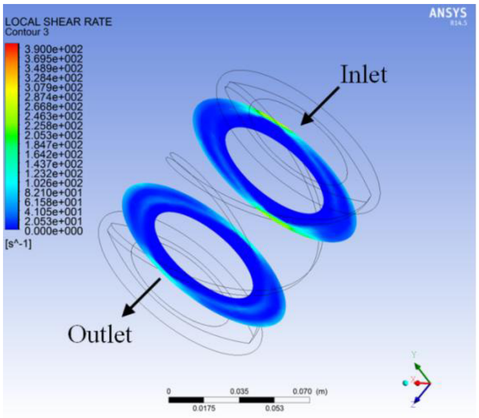

Fig. 7. Distribution of shearing rate in XY section.

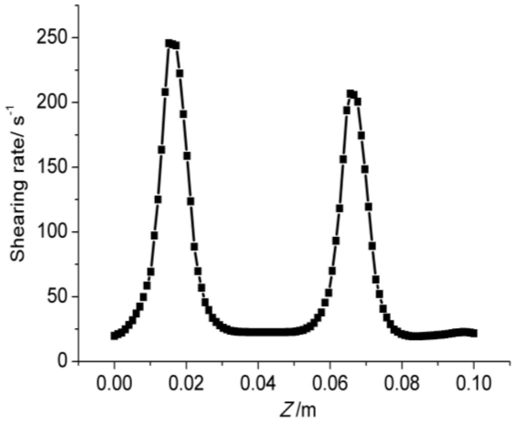

Fig. 8. Distribution of shearing rate at axial direction.

3.4. Pressure

The pressure distribution trends of GR-35 in the process of extrusion were shown in Fig. 9 and Fig. 10.

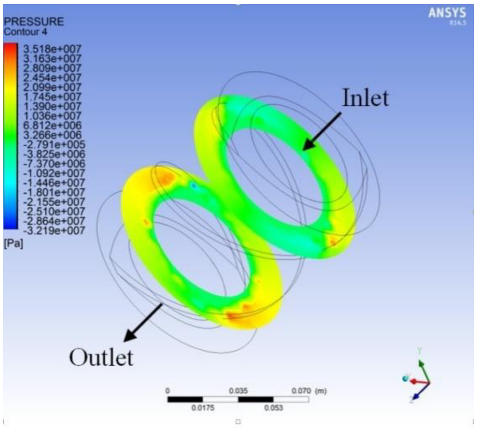

Fig. 9. Pressure distribution in XY section.

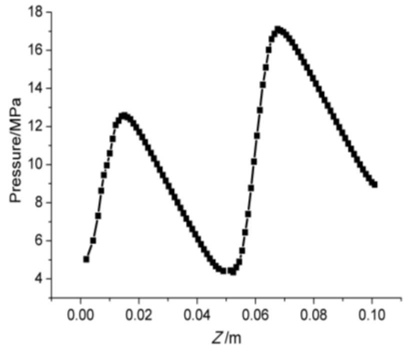

Fig. 10. Pressure distribution at axial direction.

From Fig. 9, it can be seen that the pressure varies regularly in the process of extrusion. According to Fig. 10, from the back to the front, the pressure increased at the two arrises. The maximum pressure at arris was 13 MPa and 17 MPa respectively. The phenomenon was caused by the higher propulsion at arris in the extrusion process. The higher propulsion resulted in higher extrusion force for the material. However, with the mixing of the material, it's compaction. The pressure gradually increased due to the force among materials.

4. Conclusions

In this paper, Polyflow software was used to simulate the screw process of GR-35 propellant. According the results, three conclusions can be drawn.

(1) In the extrusion forming process of double base propellant, the influence of friction and extrusion will lead to temperature rise. If the there were some errors in process conditions, it even lead to combustion and explosion.

According to the results of simulation for solid propellant, the temperature, pressure and shearing rate at screw arris were higher than other position. These phenomena mean the higher possibility for accidents.

(2) In the extrusion process of double base propellant, the temperature, pressure and shearing rate will be higher near the outlet. So not only yield but also safety should be considered in the extrusion process.

(3) It was valuable to apply Polyflow software in the extrusion process of double base propellant. It can simulate the changes of flow based on different conditions in extrusion process. The results can be used to adjust process condition for inherent safety. But this is a preliminary exploration so that more work will be done in the future.

References

[1] Suo-en Liu. Research on Characteristics Improvement of a High Energy Screw CMDB Propellant. Chinese J. Explos. Propell. 1997, 2.

[2] Xiao-jing Liu. Safety analysis and evaluation of typical production processes for explosives.Nanjing Univerisity of Science and technology. 2004.

[3] Han-cheng Deng. The Isothermal Visco-Flow Theory of Screw Extrusion for Double-Base Propellant. J. Nanjing U. Sci. Techn.(Nat. Sci.). 1980, 2: 95−106.

[4] Xin Qian, Wang-ding Xu, Yang-fu Jin. POLYFLOW foundation and its application in plastics processing.Chemical Industry Press, Beijing, 2010

[5] WilczyÄski. K. Single-screw Extrusion Model for Plasticating Extrusion.Polym-Plast. Technol. 1999(4): 581-608.

[6]Jaluria Y. Modeling and Simulation of the solids Conveying and Unfilled Regions in Polymer Extrusion. J. Reinf. Plast. Comp. 1999, 18(1): 15−26.

[7] Thompson M.R.Discrete Particle Simulation of Solid Compaction and conveying in A Single-Screw Extruder. Polym. Eng. Sci. 2008, 48(1): 62−73.

[8] Ji-yuHe, Shao-zhenChen, Jian-wuDai. The Effect Factors of the Extrudate Temperature during the Processing of Twin -screw Extruder.Chinese J. Explos. Propell.2000(1): 40−42.

[9] Xiao-qingYang, Wu-xueDing, Shuan-huWang. Simulation of casting film process based on Polyflow. Light Ind. Mach. 2011, 29(1): 16-19

[10] BinLiu, JunMa. Application of Polyflow Inverse Extrusion in the Design of Profile Die. Plast. Sci. Tech. 2008 (1): 66−70

[11] Yu-yingMa. A study on processing properties of GR-35 double base propellant. J. Propell. Tech. 1995, 16(4): 66−70.

[12] Bertrand F., Tanguy P. A., Thibault F. A three - dimensional fictitious domain method for incompressible fluid flow problems. Int. J. Numer. Meth. Fl. 1997, 25(6): 719−736.

[13] Yu-feiPang. An auto-disposal technology of overlap grid method and its application on CFD. National University of defense technology, 2005.

[14] Xing-yongSun, Jin-nanChen, JiongPeng. Three-dimensional numerical simulation of liquid in transition segment of the co-rotating twin-screw extruder. J. Petrochem. Univ.2006, 18(3): 69−71.

[15] Jia-li Yang, He-sheng Liu, Xing-yuan Huang, Lei Xu. Application of Polyflow inverse extrusion method in the design of T-shaped plastics profile extrusion die. Plast. 2011, 40(1): 114−117.

[16] Connelly R. K., Kokini J. L. Examination of the mixing ability of single and twin screw mixers using 2D finite element method simulation with particle tracking. J.Food Eng. 2007, 79(3): 956−969.